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				Welcome to DIM International
NEWS	1			Web Page for STN Seminar Schedule - N. America
NEWS	2	AUG	15	CAOLD to be discontinued on December 31, 2008
NEWS	3	OCT	07	EPFULL enhanced with full implementation of EPC2000
NEWS	4	OCT	07	Multiple databases enhanced for more flexible patent number searching
NEWS	5	OCT	22	Current-awareness alert (SDI) setup and editing enhanced
NEWS	6	OCT	22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS	7	OCT	24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances
NEWS	8	NOV	21	CAS patent coverage to include exemplified prophetic substances identified in English-, French-, German-, and Japanese-language basic patents from 2004-present
NEWS	9	NOV	26	MARPAT enhanced with FSORT command
NEWS	10	NOV	26	MEDLINE year-end processing temporarily halts
				availability of new fully-indexed citations
NEWS	11	NOV	26	CHEMSAFE now available on STN Easy
NEWS	12	NOV	26	Two new SET commands increase convenience of STN searching
NEWS	13	DEC	01	ChemPort single article sales feature unavailable
	14			GBFULL now offers single source for full-text
				coverage of complete UK patent families
NEWS	15	DEC	17	Fifty-one pharmaceutical ingredients added to PS
NEWS	EXP	RESS		E 27 08 CURRENT WINDOWS VERSION IS V8.3, CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.
NEWS	HOU LOG	OGIN W		N Operating Hours Plus Help Desk Availability Leome Banner and News Items r general information regarding STN implementation of IPC 8

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:20:31 ON 19 DEC 2008

=> index

ENTER FILE OR CLUSTER NAMES (NONE):

ENTER FILE OR CLUSTER NAMES (NONE): chem

'CHEM' IS AN AMBIGUOUS REFERENCE

- Chemical Engineering Cluster CHEMENG

CHEMISTRY - Chemical Literature Cluster
CHEMCATS - CHEMICAL CATALOGS ONLINE 1993-to the present
CHEMINFORMEX - The CHEMINFORMEX Reaction Search Service

CHEMLIST - Regulated Chemicals Listing

CHEMSAFE

- Regulaced Chemical Safety information ENTER A FILE OR CLUSTER NAME (IGNORE): chemistry

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INDEX 'AGRICOLA, ALUMINIUM, ANABSTR, APOLLIT, AQUALINE, AQUIRE, BABS, BIOTECHNO, CABA, CAPLUS, CBNB, CEABA-VTB, CERAB, CIN, COMPENDEX, CONFSCI, COPPERLIT, CORROSION, DISSABS, ENCOMPLIT, GENBANK, INSPEC, INSPHYS, IPA, KOSMET, METADEX, NAPRALERT, NTIS, ...' ENTERED AT 13:20:51 ON 19 DEC 2008

39 FILES IN THE FILE LIST IN STNINDEX

Enter SET DETAIL ON to see search term postings or to view search error messages that display as 0* with SET DETAIL OFF.

=> file reg

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0.65 0.86 FULL ESTIMATED COST

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http://www.cas.org/support/stngen/stndoc/properties.html

=> e phthalocvanine/cn

PHTHALOCYANINATOPLATINUM/CN 1

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1 PHTHALOCYANINATOZINC/CN
E2
E3
                                    1 --> PHTHALOCYANINE/CN
E4
                                   1 PHTHALOCYANINE 158 (LUBRICANT)/CN
E5
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                                                     PHTHALOCYANINE ANION/CN
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                                                    PHTHALOCYANINE ANTIMONY AMIDE/CN
E6
                           1 PHTHALOCYANINE BLUE (N
1 PHTHALOCYANINE BLUE 01216/CN
1 PHTHALOCYANINE BLUE 1570/CN
1 PHTHALOCYANINE BLUE 1573/CN
1 PHTHALOCYANINE BLUE 4044/CN
1 PHTHALOCYANINE BLUE 4170/CN
E7
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1 PHTHALOCYANINE BLUE 4982/CN
1 PHTHALOCYANINE BLUE 5240K/CN
1 PHTHALOCYANINE BLUE AFT 9650/CN
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1 PHTHALOCYANINE BLUE BT
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1 PHTHALOCYANINE BLUE BT
465D/CN
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1 PHTHALOCYANINE BLUE SG/CN
1 PHTHALOCYANINE BLUE SG/CN
1 PHTHALOCYANINE BLUE WDB 4675/CN
1 PHTHALOCYANINE BLUE ZC 907/CN
1 PHTHALOCYANINE BLUE MDB 4675/CN
1 PHTHALOCYANINE BLILLIANT GREEN/CN
1 PHTHALOCYANINE COBALT/CN
1 PHTHALOCYANINE COBALT COMPLEX/CN
1 PHTHALOCYANINE COBALT COMPLEX/CN
1 PHTHALOCYANINE DIANION/CN
1 PHTHALOCYANINE DIANION/CN
1 PHTHALOCYANINE DIANION/CN
1 PHTHALOCYANINE OF 1051/CN
1 PHTHALOCYANINE GREEN/CN
E25
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1 PHTHALOCYANINE GREEN 2GN/CN
1 PHTHALOCYANINE GREEN 2GN/CN
1 PHTHALOCYANINE GREEN 6G/CN
1 PHTHALOCYANINE GREEN 6TH/CN
1 PHTHALOCYANINE GREEN 6TH/CN
1 PHTHALOCYANINE GREEN 6ZH/CN
1 PHTHALOCYANINE GREEN G/CN
1 PHTHALOCYANINE GREEN G/CN
1 PHTHALOCYANINE GREEN GTP/CN
1 PHTHALOCYANINE GREEN LX/CN
1 PHTHALOCYANINE GREEN LX/CN
1 PHTHALOCYANINE GREEN NY/CN
1 PHTHALOCYANINE GREEN NY/CN
E37
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                                 1 PHTHALOCYANINE GREEN V/CN
1 PHTHALOCYANINE GREEN VFT 1080/CN
E49
E50
                                  1 PHTHALOCYANINE GREEN WDG 47/CN
1 PHTHALOCYANINE IRON/CN
1 PHTHALOCYANINE LIGHT BLUE VK/CN
E51
E52
E53
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E54
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E55
             1
                  PHTHALOCYANINE LIGHT FAST YELLOW 4K/CN
E56
                  PHTHALOCYANINE POLYMER/CN
             1
E57
             1
                  PHTHALOCYANINE PV FAST ORANGE/CN
            1 PHTHALOCYANINE RADICAL CATION/CN
1 PHTHALOCYANINE RADICAL CATION/CN
1 PHTHALOCYANINE RADICAL ION(1-)/Cl
E58
E59
E60
                  PHTHALOCYANINE RADICAL ION(1-)/CN
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E61
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                  PHTHALOCYANINE RED/CN
E62
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                   MPLEX/CN
                  PHTHALOCYANINE TURQUOISE BLUE/CN
E63
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             1
                  PHTHALOCYANINE VIOLET/CN
E64
E65
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                   TRIAZINE-2, 4-DIYL) DIIMINO) DI-/CN
E66
            1
                  PHTHALOCYANINE, (2-CHLOROACETAMIDOMETHYL) -, CU DERIV./CN
E67
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                  PHTHALOCYANINE, (ACETOACETAMIDOMETHYL) -, CU DERIV./CN
                PHTHALOCYANINE, (BROMOMETHYL)-, CU DERIV./CN PHTHALOCYANINE, (CHLOROMETHYL)-/CN
E68
             1
E69
            1
            PHTHALOCYANINE, (CHLOROMETHYL)-, CU DERIV./CN
PHTHALOCYANINE, (PHENTLSUIGNYL)-, CO DERIV./CN
PHTHALOCYANINE, , PBIS (DODECYLOXY)-14,15-BIS (2-(2-(2-МЕТНОХҮЕ
E70
E71
E72
                   THOXY) ETHOXY) ETHOXY) -/CN
=> e
E73
             1
                  PHTHALOCYANINE, 10-PROPOXY-/CN
E74
                  PHTHALOCYANINE, 12,13-BIS((4-(1,1-DIMETHYLETHYL)PHENYL)THIO)
            1
                   -/CN
E75
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                  PHTHALOCYANINE, 14,15-DIHEXADECYL-,-BIS(HEXADECYLOXY)-,-BIS(
                   2-(2-(2-METHOXYETHOXY) ETHOXY) ETHOXY) -/CN
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                   PHTHALOCYANINE, 2,10,16,24-TETRAKIS(TRIMETHYLSILYL)-/CN
E76
E77
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                   PHTHALOCYANINE, 2,3-BIS(2-(2-METHOXYETHOXY)ETHOXY)-/CN
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E78
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                  PHTHALOCYANINE, 2,5-BIS(4-(HEXYLOXY)PHENOXY)-/CN
                  PHTHALOCYANINE, 20,23,25,28-TETRAOCTYL-12-(4-(TRICHLOROSILYL
E80
            1
                   )BUTOXY)-/CN
                  PHTHALOCYANINE, 4,4',4'',4'''-TETRAMETHOXY-, CO DERIV./CN
E81
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E82
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                  PHTHALOCYANINE, 4-(DODECYLOXY)-5-(2-(2-(2-METHOXYETHOXY)ETHO
                   XY) ETHOXY) -/CN
E83
            1
                  PHTHALOCYANINE, 5,6-BIS(DODECYLOXY)-,-BIS(2-(2-(2-METHOXYETH
                   OXY) ETHOXY) ETHOXY) -/CN
E84
            1
                  PHTHALOCYANINE, 5,6-BIS(HEXYLTHIO)-, CONJUGATE ACID (1:2)/CN
=> s e3
             1 PHTHALOCYANINE/CN
T. 1
=> d scan
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L1 1 ANSWERS REGISTRY OF STREET OF STREET



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=> s 11 L2 8782 L1

L2 8/82 L

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```
=> d l1 1 ide
L1
    ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 574-93-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN 29H, 31H-Phthalocvanine (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Phthalocvanine (8CI)
OTHER NAMES:
CN x-Phthalocyanine
CN 29H, 30H-Tetrabenzo[b, g, 1, q]porphine
CN 5,28:14,19-Diimino-7,12:26,21-
    dinitrilotetrabenzo[c,h,m,r][1,6,11,16]tetraazacvcloeicosine
CN
    8120S
CN Blue Pigment B
CN C.I. 74100
CN C.I. Pigment Blue 16
CN CG 1-1
CN Fastogen Blue 8110
CN Fastogen Blue 8120
CN Fastogen Blue 8120B
CN Fastogen Blue 8120BS
CN Fastogen Blue GS
CN Heliogen Blue 7560
CN Heliogen Blue 7800
CN Heliogen Blue D 7490
CN Heliogen Blue D 7560
CN
    Heliogen Blue D 7565
CN Heliogen Blue G
CN Heliogen Blue L 7460
CN Heliogen Blue L 7560
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CN Heliogen Blue LG

Liophoton

Irgalite Blue GLS

Irgazin Blue 3GT

Lionol Blue KW

CN

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CN
    Liophoton THP
CN Liophoton TPA 891
CN MCP 80
CN
    Monastral Fast Blue G
CN
    Monolite Fast Blue GS
CN
    NA 570
    PB 16
CN
CN Photo Fine TPA 891
CN Pigment Blue 16
CN Pigment Blue Green Phthalocyanine U
CN Polymon Blue G
    Progen I
CN
CN
    PV-Fast Blue G
    Tetrabenzoporphyrazine
CN
    Tetrabenzotetraazaporphine
CN
CN Tetrabenzo[b,g,l,q]porphine
CN
    Tetrabenzo[b,g,1,q]porphyrazine
CN
    TPA 891
CN
    Vulcafor Fast Blue G
CN
    Vulcanosine Fast Bremen Blue G
CN
    Vvnamon Blue G
DR
    889688-86-2, 162831-66-5, 2612-54-6, 81612-16-0, 4466-64-2, 52440-51-4
MF
    C32 H18 N8
CI
    COM, RPS
T.C
    STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, BIOTECHNO,
       CA, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST,
       CIN, CSCHEM, CSNB, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2,
       GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, PIRA, PROMT,
       SPECINFO, TOXCENTER, TULSA, USPAT2, USPATFULL, USPATOLD
        (*File contains numerically searchable property data)
     Other Sources: DSL**, EINECS**, TSCA**
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8782 REFERENCES IN FILE CAPLUS (1907 TO DATE)
8 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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```
=> s 11 and metal
          8782 L1
       1888457 METAL
        940767 METALS
       2286478 METAL
                 (METAL OR METALS)
L3
          3519 L1 AND METAL
=> s 13/prep
          8782 L1
             0 METAL/CT
       4691145 PREP/RL
             0 METAL/PREP
                  (METAL/CT (L) PREP/RL)
L4
             0 (L1 AND METAL/PREP)
=> s l1/prep
          8782 L1
       4691145 PREP/RL
L5
           998 L1/PREP
                 (L1 (L) PREP/RL)
=> s 15 and phthalonitrile
          2233 PHTHALONITRILE
           340 PHTHALONITRILES
          2328 PHTHALONITRILE
                  (PHTHALONITRILE OR PHTHALONITRILES)
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           156 L5 AND PHTHALONITRILE
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'AND' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'
'ALKOXY' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'
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BIB ----- AN, plus Bibliographic Data and PI table (default)
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
CLASS ----- IPC, NCL, ECLA, FTERM
DALL ---- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
             SCAN must be entered on the same line as the DISPLAY,
             e.g., D SCAN or DISPLAY SCAN)
STD ---- BIB, CLASS
IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels
OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels
SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations
HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
            containing hit terms
HITRN ----- HIT RN and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
            its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
            structure diagram, plus NTE and SEQ fields
FHITSTR ---- First HIT RN, its text modification, its CA index name, and
            its structure diagram
FHITSEQ ---- First HIT RN, its text modification, its CA index name, its
            structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs
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=> s 15 and alkoxy
125108 ALKOXY
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7 ALKOXIES 125114 ALKOXY

(ALKOXY OR ALKOXIES)

L7 25 L5 AND ALKOXY

=> d scan ti hit

- L7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
 - I Gamma- or modified gamma metal-free phthalocyanines
- IT 91-15-6 1313-82-2, uses and miscellaneous 3001-72-7 3468-11-9 6674-22-2 22780-52-5D, alkoxy derivs. 51301-54-3 RL: USES (USes)

(in gamma-phthalocyanine manufacture)

11 5/9-3

RL: PREP (Preparation)

(y-form, manufacture of, seed crystals for)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Process and apparatus for preparing metal or nonmetal phthalocyanine without solvent
- T 574-93-6DF, Phthalocyanine, of metal or nonmetal phthalocyanine RL: SPN (Synthetic preparation), PREP (Freparation) (preparation of metal or nonmetal phthalocyanine)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Near-IR absorbent for electrophotographic toner and electrophotographic toner containing same
- 132-16-1DP, reaction products with 2,3 fused 1,4-benzothiazines, derivs. with 2-aminoalkyl sulfophenyls 147-14-8DP, reaction products with 2,3 fused 1,4-benzothiazines, derivs. with 2-aminoalkyl sulfophenyls 147-14-8DP, reaction products with 2.3 fused 1.4-benzothiazines, derivs. with 2-aminoalkyl sulfophenyls, chloro and fluoro 147-14-8DP, reaction products with 2.3 fused 1.4-benzothiazines, derivs, with chloro and 2-aminoalkyl sulfophenyls 574-93-6DP, 29H,31H-Phthalocyanine, reaction products with 2,3 fused 1,4-benzothiazines, derivs. with 2-aminoalkyl sulfophenyls 3317-67-7DP, reaction products with 2,3 fused 1,4-benzothiazines, derivs. with 2-aminoalkyl sulfophenyls 13930-88-6DP, reaction products with 2,3 fused 1,4-benzothiazines, derivs. with 2-aminoalkyl sulfophenyls 14154-42-8DP, reaction products with 2,3 fused 1,4-benzothiazines, derivs, with 2-aminoalkyl sulfophenyls 14320-04-8DP, reaction products with 2,3 fused 1,4-benzothiazines, derivs. with 2-aminoalkyl sulfophenyls 20909-39-1DP, reaction products with 2,3 fused 1,4-benzothiazines, derivs. with 2-aminoalkyl sulfophenyls 26201-32-1DP, reaction products with 2,3 fused 1,4-benzothiazines, derivs. with 2-aminoalkyl sulfophenyls RL: MOA (Modifier or additive use); PNU (Preparation, unclassified); TEM (Technical or engineered material use); PPEP (Preparation); USES

(Uses)
 (electrophotog. toner containing phthalocyanine aminothiophenol derivs. as near-IR absorbent)

- L7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Method for producing 1,3-diiminoisoindoline derivatives
- IT 574-93-60P, Phthalocyanine, derivs.
- RL: PNU (Preparation, unclassified); PREP (Preparation)

(preparation of 1,3-diiminoisoindoline derivs. as coloring components for thermal recording materials and precursors of phthalocyanines)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Electrophotographic photoreceptor containing poly-N-vinylcarbazole and hydrazone for optical printers
- IT 574-93-6P, Phthalocyanine 23627-89-6P, Naphthalocyanine 26201-32-1P, Titanylphthalocyanine 68105-27-1P 136424-43-6P RL: PREP (Preparation)
 - (preparation of, as charge-generating material for electrophotog. photoreceptor)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Monolayer-forming substituted phthalocyanine compounds
- IT 574-93-68, 29H,31H-Phthalocyanine 77474-65-8P 83484-76-8DP, bismuth complex 83484-76-8P 91083-54-4P 93530-42-8P 93530-45-1P 93530-46-2P 93530-47-3P 93530-48-4P 93530-49-5P 93530-50-8P

103696-21-5P 103714-74-5P 103804-66-6P

RL: PREP (Preparation)

(preparation of, as monolayer-forming semiconductor films)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Eta or modified eta metal-free phthalocyanines
- IT 91-15-6 3001-72-7 3468-11-9 6674-22-2 22780-52-5D, alkoxy derivs. 25566-72-7 27755-14-2 40795-63-9 51301-54-3 RL: USES (Uses)
 - (in eta-phthalocyanine manufacture)
- IT 574-93-6P
 - RL: PREP (Preparation)

 $(\eta-form, manufacture of)$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Phthalocyanine synthesis in ionic liquids: Preparation of differently substituted phthalocyanines in tetrabutylammonium bromide
- IT Substitution reaction, nucleophilic
 - (preparation of alkoxy and phenoxy phthalonitrile derivs. by nucleophilic substitution reaction using phthalonitriles and alcs., phenol, alkyl bromide, mercapto alkanes as reactants and molten tetrabutylammonium bromide (ionic liquid) as solvent)
- IT Alcohols, reactions

Thiols, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of alkoxy and phenoxy phthalonitrile derivs. by nucleophilic substitution reaction using phthalonitriles and alcs., phenol, alkyl bromide, mercapto alkanes as reactants and molten tetrabutylammonium bromide (ionic liquid) as solvent)

- IT 108-95-2, Phenol, reactions 111-87-5, 1-Octanol, reactions 629-04-9, Heptyl bromide 4733-50-0, 3,6-Dihydroxyphthalonitrile RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of alkoxy and phenoxy phthalonitrile derivs. by
 - (preparation or alkox; and paenoxy partnations are derives, by nucleophilic substitution reaction using phthalonistrile derivs, and alcs., phenol, or alkyl bromide as starting materials and molten tetrabutylammonium bromide (ionic liquid) as solvent)
- IT 106144-21-2P, 4-Octoxy-1,2-benzenedicarbonitrile
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 - (preparation of alkozy and phenoxy phthalonitrile derivs. by nucleophilic substitution reaction using phthalonitrile derivs. and alcs., phenol, or alkyl bromide as starting materials and molten tetrabutylammonium bromide (ionic liquid) as solvent)
- II 116453-88-1P 147699-63-6P, 4,5-Diphenoxyphthalonitrile 696614-51-4P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of alkoxy and phenoxy phthalonitrile derive. by
- nucleophilic substitution reaction using phthalonitrile derivs. and alcs., phenol, or alkyl bromide as starting materials and molten tetrabutylammonium bromide (ionic liquid) as solvent)

 T 574-93-6DP, Phthalocyanine, derivs. 140141-44-2P 140161-62-2P
- 165284-84-4P 177991-94-5P 439812-66-5P 858675-24-8P 858675-25-9P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of phthalocyanine derive. by cyclization using phthalonitrile derive. as reactants and molten tetrabutylammonium bromide (ionic liquid) as solvent)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Electrophotographic photoreceptor using tetraazaporphyrin derivatives
- IT 147-14-8P 574-93-6P, 29H, 31H-Phthalocyanine 1661-03-6P
 - 24724-50-3P 26201-32-1P 54398-42-4P 75069-95-3P 75087-14-8P
 - 108187-01-5P 265654-33-9P 288847-46-1P 288847-47-2P 288850-86-2P
 - 288850-87-3P 288850-88-4P 288850-89-5P 288850-90-8P 288850-91-9P 288850-92-0P 288850-93-1P
 - RL: DEV (Device component use); PNU (Preparation, unclassified); FREP (Preparation); USES (Uses)
 - (electrophotog. photoreceptor containing tetraazaporphyrin compds. as charge-generating agent)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Preparation of phthalonitrile compounds as phthalocyanine intermediates
- IT 574-93-6P, Phthalocyanine
- RL: PNU (Preparation, unclassified); PREP (Preparation)
 - (preparation of phthalonitriles as phthalocyanine intermediates from nitrophthalonitrile and dithiocarbamates)
- HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):
- HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1
- L7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Process for preparation of silicon-phthalocyanine compounds by reaction of diminoisoindolines with silicon tetrachloride
- IT 574-93-6DF, Phthalocyanine, silicon dihydroxide complexes 19333-15-4P 85214-70-6P 92396-90-2P 152248-88-9P 154293-21-7P 15989-00-5P 159539-84-1P 159539-85-2P 159539-86-3P 159539-87-4P 159539-88-5P 159539-89-6P

RL: DEV (Device component use); IMF (Industrial manufacture); FREP

(Preparation); USES (Uses)

(process for preparation of silicon-phthalocvanine compds. by reaction of diiminoisoindolines with silicon tetrachloride in presence of DBU)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- Electrophotographic photoreceptors using phthalocyanine derivative and TI hydrazone-containing styrene copolymer
- ΙT 574-93-6P, Phthalocvanine 23627-89-6P

RL: PPEP (Preparation)

(preparation of, charge-generating agent, electrophotog, photoreceptor using, with titanyl phthalocyanine)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- T. 7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- ΤI Hydrazone compounds for electrophotographic photoreceptors
- ΙT 574-93-6P, Phthalocyanine 92888-89-6P 96222-86-5P
- 103079-12-5P 103079-13-6P 103079-14-7P 106200-80-0P RL: IMF (Industrial manufacture); PREP (Preparation)

(preparation of, for photoreceptor photoconductive coatings)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Dve-containing hardenable material composition with azaporphyrin for manufacturing color filters for optical imaging device
- TT 574-93-6DP, Phthalocyanine, aza containing alkoxy amino

sulfonyl substituted copper complexes 7440-50-8DP, Copper, complex with phthalocyanine, aza containing, sulfonyl amino alkyl substituted

852162-90-4P 852162-92-6P 852162-94-8P 852162-96-0P 852162-98-2P 852163-00-9P 852163-02-1P 852163-04-3P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREF (Preparation); USES (Uses)

(azaporphyrin in hardenable material composition)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L7 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- Preparation of metallocyclopentadienyl derivatives of phthalocyanine for TΙ use in optical information storage applications
- 574-93-6DP, Phthalocyanine, derivs. 821867-96-3P 821868-11-5P
 - 821868-44-4P 821868-84-2P 821869-11-8P 821869-27-6P 821869-35-6P 821869-58-3P 821869-82-3P 821869-96-9P 821870-11-5P 821870-29-5P 821870-51-3P 821870-66-0P 821870-81-9P 821870-97-7P 821871-05-0P

821871-20-9P 821871-35-6P 821871-50-5P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of phenylmetallocyclopentadienyl phthalocyanine derivs. for optical information storage)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
- TI Purification of alkoxyphthalocyanine derivatives
- 574-93-6DP, Phthalocyanine, alkoxy derivs.

216018-34-7DP, brominated 216018-35-8P 216018-36-9P RL: PUR (Purification or recovery); PREP (Preparation)

```
(dissoln. in organic solvents and adsorption onto silica gels in
purification
        of alkoxyphthalocvanine derivs.)
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1
     25 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
L7
    Production of metal-free phthalocyanines.
TΙ
    574-93-6DP, Phthalocyanine, chloro derivs, 574-93-6P,
     Phthalocvanine
     RL: IMF (Industrial manufacture); PREF (Preparation)
        (production of metal-free phthalocvanines)
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0
=> s 11 and metal-containing
         8782 I.1
       1888457 METAL
        940767 METALS
       2286478 METAL
                 (METAL OR METALS)
        696577 CONTAINING
             3 CONTAININGS
        696580 CONTAINING
                 (CONTAINING OR CONTAININGS)
       4290904 CONTG
            38 CONTGS
       4290916 CONTG
                 (CONTG OR CONTGS)
       4493882 CONTAINING
                 (CONTAINING OR CONTG)
         22430 METAL-CONTAINING
                 (METAL (W) CONTAINING)
L8
            79 L1 AND METAL-CONTAINING
=> s 18/prep
          8782 L1
             0 METAL-CONTAINING/CT
       4691145 PREP/RL
             0 METAL-CONTAINING/PREP
                 (METAL-CONTAINING/CT (L) PREP/RL)
L9
             0 (L1 AND METAL-CONTAINING/PREP)
=> s 18 and phthalonitrile
          2233 PHTHALONITRILE
           340 PHTHALONITRILES
          2328 PHTHALONITRILE
                 (PHTHALONITRILE OR PHTHALONITRILES)
L10
             6 L8 AND PHTHALONITRILE
=> s 18 and (phthalonitrile OR "1,2-Benzenedicarbonitrile" OR "1,2-Dicyanobenzene"
OR "Phthalodinitrile")
          2233 PHTHALONITRILE
           340 PHTHALONITRILES
          2328 PHTHALONITRILE
                 (PHTHALONITRILE OR PHTHALONITRILES)
       9930505 "1"
       9870720 "2"
           778 "BENZENEDICARBONITRILE"
            28 "BENZENEDICARBONITRILES"
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786 "BENZENEDICARBONITRILE"
                ("BENZENEDICARBONITRILE" OR "BENZENEDICARBONITRILES")
          453 "1,2-BENZENEDICARBONITRILE"
                ("1"(W)"2"(W)"BENZENEDICARBONITRILE")
      9930505 "1"
      9870720 "2"
         1388 "DICYANOBENZENE"
          136 "DICYANOBENZENES"
         1447 "DICYANOBENZENE"
                 ("DICYANOBENZENE" OR "DICYANOBENZENES")
          353 "1,2-DICYANOBENZENE"
                ("1"(W)"2"(W)"DICYANOBENZENE")
          531 "PHTHALODINITRILE"
           44 "PHTHALODINITRILES"
          550 "PHTHALODINITRILE"
                ("PHTHALODINITRILE" OR "PHTHALODINITRILES")
            7 L8 AND (PHTHALONITRILE OR "1,2-BENZENEDICARBONITRILE" OR "1,2-DI
              CYANOBENZENE" OR "PHTHALODINITRILE")
=> d ibib hit hitstr
L11 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        2006:992382 CAPLUS Full-text
DOCUMENT NUMBER:
                        147:156524
TITLE:
                        Low-temperature synthesis of phthalocyanine and its
                        metal complexes
                        Kharisov, B. I.; Ortiz Mendez, U.; Rivera de la Rosa,
AUTHOR(S):
                        J.
CORPORATE SOURCE:
                       Institute of Physical Chemistry, Russian Academy of
                        Sciences, Moscow, 119991, Russia
SOURCE:
                        Russian Journal of Coordination Chemistry (2006),
                        32(9), 617-631
                        CODEN: RJCCEY; ISSN: 1070-3284
PUBLISHER:
                        Pleiades Publishing, Inc.
DOCUMENT TYPE:
                        Journal
LANGUAGE:
                       English
OTHER SOURCE(S):
                        CASREACT 147:156524
     Conditions for synthesizing unsubstituted phthalocyanine and its metal
     complexes from phthalonitrile at low temps. (0-50°) are optimized.
     Phthalocyanine and phthalocyaninates are produced under these conditions using
     activated Rieke metals, metals on inert substrate, sources of soluble metals
     as unstable metal complexes, zeolites, solid-phase electrosynthesis of
     phthalonitrile, and UV irradiation. The use of pyrophoric metals is the most
     efficient due to a large number of defects in their structure favoring the
     initial stage of phthalonitrils cyclization on a metal matrix. The suggested
     mechanism of formation of phthalocyanine macrocycle assumes participation of
     metal agglomerates occurring in activated metals.
    Zeolites (synthetic), reactions
    RL: RCT (Reactant); RACT (Reactant or reagent)
       (metal containing; for low-temperature preparation of metal
       phthalocyaninates)
    147-14-8P, Phthalocyaninatocopper 574-93-6P, Phthalocyanine
    1661-03-6P, Phthalocyaninatomagnesium 14055-02-8P 14320-04-8P,
    Phthalocyaninatozinc 15187-16-3P, Phthalocyaninatolead 21328-74-5P,
    Phthalocyaninatocadmium
    RL: SPN (Synthetic preparation); PREP (Preparation)
       (optimization of low-temperature preparation of)
    91-15-6, Phthalonitrile 7439-95-4, Magnesium, reactions
    7440-02-0, Nickel, reactions 7440-43-9, Cadmium, reactions 7440-50-8,
    Copper, reactions 7440-66-6, Zinc, reactions
```

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant for low-temperature preparation of metal phthalocyaninate)

IT 574-93-6P, Phthalocyanine

RL: SPN (Synthetic preparation); PREP (Preparation) (optimization of low-temperature preparation of)

RN 574-93-6 CAPLUS

CN 29H, 31H-Phthalocyanine (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L11 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:1014304 CAPLUS Full-text

41

DOCUMENT NUMBER: 142:8099

TITLE: Substituted phthalocyanine compounds with excellent solubility, color tone, and fastness, their

preparation, inks from them, and ink-jet recording

method using them

INVENTOR(S): Tateishi, Keiichi; Tanaka, Shigeaki

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 59 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|----------|-----------------|----------|
| | | | | |
| JP 2004331734 | A | 20041125 | JP 2003-126442 | 20030501 |
| PRIORITY APPLN. INFO.: | | | JP 2003-126442 | 20030501 |
| OTHER SOURCE(S): | MARPAT | 142:8099 | | |

B The compds. MPc(SO2L1R1)k(SO2L2R2)mR3n [A; M = H, metal, oxide, hydroxide, halogenated compound; M-Pc = phthalocyanine core with valence of (k + m + n); L1,2 = divalent linking group; R1,2 = substituent; R3 = H, substituent; ≥1 of R1-3 = ionic hydrophilic group; k, n >0 but <16; m ≥0 but <16; k + m + n = 16] are prepared by reacting (SO2L1R1)q-containing cyclic compds. (q = 1-2; L1, R1 = same as above), (SO2L2R3)p-containing cyclic compds. (p = 1-4; L2, E2 = same as above), and/or R3r-containing cyclic compds. (r = 0-4; R3 = same as above) and metal derivs. MXd (M = same as above; X = mono- or divalent ligand; d = 0-4) in buffers from alkali metal-containing (organic) bases and acids. Thus, a storage-stable ink containing a Cu phthalocyanine dye mixture (A; M = Cu; L1 = (CH2)3; R1 = SO3Li; R3 = H; k = 3; m = 0; n = 1) prepared from 4-

nitrophthalimide and o-phthalonitrile gave an image with good water, light, and ozone resistance.

147-14-8D, Copper phthalocyanine, derivs. 574-93-6D,

Phthalocyanine, derivs.

RL: TEM (Technical or engineered material use); USES (Uses)

(cyan dye; preparation of substituted phthalocyanine dyes for ink-jet inks with good storage stability and light, water, and ozone resistance)

89-40-7, 4-Nitrophthalimide 91-15-6, o-Phthalonitrile

RL: RCT (Reactant); RACT (Reactant or reagent)

(for dve preparation; preparation of substituted phthalocvanine dves for ink-jet

inks with good storage stability and light, water, and ozone resistance)

574-93-6D, Phthalocyanine, derivs.

RL: TEM (Technical or engineered material use); USES (Uses)

(cyan dye; preparation of substituted phthalocyanine dyes for ink-jet inks with good storage stability and light, water, and ozone resistance)

RM 574-93-6 CAPLUS

29H, 31H-Phthalocvanine (CA INDEX NAME) CN

L11 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1992:48861 CAPLUS Full-text

DOCUMENT NUMBER: 116:48861

ORIGINAL REFERENCE NO.: 116:8287a,8290a

TITLE: Electrophotographic photoconductors

INVENTOR(S): Matsui, Naovuki; Goto, Tomohisa

PATENT ASSIGNEE(S): NEC Corp., Japan

SOURCE: Jpn. Kokai Tokkvo Koho, 15 pp.

> CODEN: JKXXAF Patent

DOCUMENT TYPE: LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------------|----------|
| | | | | |
| JP 03166547 | A | 19910718 | JP 1989-304920 | 19891127 |
| PRIORITY APPLN. INFO.: | | | JP 1989-304920 | 19891127 |
| and the second of the second o | | | and the second second | |

Title photoconductors have a photosensitive layer contg. hydrazones I, butadienes II, and oxadiazoles III (R1 = H, alkyl, alkoxy, halo, amino, morpholino, piperidino, carbazoly1; R2 = H, alkyl, alkoxy, aralkyloxy, R3-4 = H, alkyl, aryl, aralkyl, pyridyl, pyrrolidinyl, carbazolyl; R5-6 = alkyl; R9-10 = H, alkyl, acyl, cycloalkyl). The photoconductors may contain chargegenerating agents of ≤50 parts metal-free or metal-containing (substituted) phthalocyanines or naphthalocyanines or their aza analogs, and 100 parts titanyl phthalocyanine, and are in crystalline form having characteristic IR

peaks at 1490±2 cm-1, 1415±2 cm-1, 1332±2 cm-1, 1119±2 cm-1, 1072±2 cm-1, 1060±2 cm-1, 961±2 cm-1, 893±2 cm-1, 780±2 cm-1, 751±2 cm-1, and 730±2 cm-1, and contain charge-transporting agents I, II and III. Thus, titanyl phthalocyanine was prepared by reaction of 20.4 parts o-phthalodinitrile and 7.6 parts TiCl4. A nonmetal phthalocyanine was prepared by heating aminoisoindolenine in quinoline. A uniform mixture of 1 part titanyl phthalocyanine with 0.05 part nonmetal phthalocyanine was prepared by precipitation from H2SO4/water/THF. An Al-coated polyester film was coated with a charge-generating layer containing the phthalocyanine mixture and poly(vinvl butyral), and then with a charge-transporting layer containing pdiethylaminobenzaldehyde diphenylhydrazone 20, 1,1-bis(p-diethylaminophenyl)-4,4-diphenyl-1,3- butadiene 60, 2,5-bis(4-diethylaminophenyl)-1,3,4-oxadiazole 20, and polycarbonate 100 parts. Obtained photoconductor was chargeable to 730 V, and showed initial dark decay to 90%, sensitivity (lux-s required for half decay of voltage) 0.5, and residual voltage 70 V. After 1000 chargingphotodischarging cycles, the photoconductor was chargeable to 700 V, dark decay to 88%, and residual voltage 70 V.

IT 574-93-6, Phthalocyanine 23627-89-6, Naphthalocyanine 26201-32-1, Titanyl phthalocyanine

RL: USES (Uses)

(electrophotog. photoconductor containing)

T 7550-45-0, Titanium tetrachloride, reactions RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with phthalodinitrile, charge-generating agents

for electrophotog. photoconductors from)

T 91-15-6, 1,2-Benzenedicarbonitrile

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with titanium tetrachloride, charge-generating agents for electrophotog. photoconductors from)

IT 574-93-6, Phthalocyanine

RL: USES (Uses)

(electrophotog. photoconductor containing)

RN 574-93-6 CAPLUS

CN 29H,31H-Phthalocyanine (CA INDEX NAME)



L11 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1976:75156 CAPLUS Full-text DOCUMENT NUMBER: 84:75156

ORIGINAL REFERENCE NO.: 84:12347a,12350a

TITLE: Colored and thermoresistant polyoxyphenylene and its

mixes with other thermo-plastics

INVENTOR(S): Penczek, Irena; Bialy, Jan; Jaczewska, Teresa;

Rafalowicz, Teodor

PATENT ASSIGNEE(S): Instytut Chemii Przemyslowej, Pol.

SOURCE: Pol., 3 pp.

CODEN: POXXA7

DOCUMENT TYPE: Patent LANGUAGE: Polish

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

AB Phthalocyanines and/or phthalonitriles were used as stabilizers and dyes of polyoxyphenylene polymers containing small amts. of metals to give heat-resistant plastics. For example, poly(2,6-dimethyl-1,4-oxyphenylene) [24938-67-8] containing 0.01% Cu [7440-50-8] 100, 2-dinaphthyl-p-phenylenediamine [93-46-9] 0.5, metal-free phthalocyanine [574-93-6] 0.08, Cu phthalocyanine [147-14-8] 0.02, and Ti white 0.3 weight parts were homogenized and molded at 300° to give a green product.

ST copper phthalocyanine stabilizer polyoxyphenylene; polyphenylene oxide stabilizer phthalocyanine; heat resistant polyphenylene oxide; metal stabilizer polyphenylene oxide; phthalonitriie stabilizer polyphenylene oxide; dye phthalocyanine polyphenylene oxide; coloring phthalocyanine polyphenylene oxide

IT 147-14-8 574-93-6

RL: USES (Uses)

(dye-stabilizers, for copper-containing polyoxyphenylenes)

IT 93-46-9

RL: USES (Uses)

(stabilizers, containing phthalocyanines, for metal-contg

. polyoxyphenylenes)

IT 574-93-6

RL: USES (Uses)

(dye-stabilizers, for copper-containing polyoxyphenylenes)

RN 574-93-6 CAPLUS

CN 29H, 31H-Phthalocyanine (CA INDEX NAME)



L11 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1971:127519 CAPLUS Full-text

DOCUMENT NUMBER: 74:127519

ORIGINAL REFERENCE NO.: 74:20585a,20588a

TITLE: Catalytic synthesis of metal-free phthalocyanine

AUTHOR(S): Twigg, M. V.

CORPORATE SOURCE: Erindale Coll., Univ. Toronto, Toronto, ON, Can. SOURCE: Organic Preparations and Procedures International

(1971), 3(2), 97-8

CODEN: OPPIAK; ISSN: 0030-4948

DOCUMENT TYPE: Journal LANGUAGE: English

- AB A mixt. of 15.2 g phthalopitrile, 1 ml cyclohexylamine, and 38 ml 1methylnaphthalene (I) was heated at 230° for 10 hr to give 10.1 g crystalline, metal-free phthalocyanine, avoiding the need for the preparation of a metalcontaining intermediate. 1-Chloronaphthalene, o-C6H4C12, or a similar solvent can be substituted for I.
- phthalocyanine metal-free; phthalonitrile polycondensation; cyclohexylamine catalyst phthalocyanine; catalyst phthalocyanine prepn

574-93-6P RL: SPN (Synthetic preparation); PREP (Preparation) (catalytic synthesis of)

574-93-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (catalytic synthesis of)

RN 574-93-6 CAPLUS

29H, 31H-Phthalocyanine (CA INDEX NAME) CN



L11 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1956:46819 CAPLUS

DOCUMENT NUMBER: 50:46819

ORIGINAL REFERENCE NO.: 50:9029d-i,9030a Basic phthalonitrile derivatives TITLE:

PATENT ASSIGNEE(S): J. R. Geigy A.-G. DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

AR

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|----------|
| | | | | |
| GB 737413 | | 19550928 | GB 1953-4245 | 19530216 |

Basic phthalonitrile derivatives TΙ

Colorless to weakly vellowish phanalonitrile (I) derivs, are converted by heat into metal-containing phthalocyanine dyes. To a 25% solution 130 of HBr in AcOH, I 12.8 parts is added at room temperature while stirring. The temperature quickly rises to 35-40° and a thicker suspension results. After a few hrs. the white precipitate is separated, washed with petr. ether, and dried in vacuo over NaOH. The product 33-35 parts, decomposing at 200-15°, has the formula C8H7N2Br3 (II) and is more stable than the known imino halides of benzene mononitriles. II 37.1 is gradually added to concentrated NH4OH 150 parts. A strong exothermic reaction takes place. After a few min. the yellow precipitate is filtered off and washed with a little H2O. From the filtrate the excess NH3 is removed to give an addnl. precipitate Combined with the above it is dried in vacuo to give C16H19O2N6Br (III) 17-19 parts. It splits off NH3 at 130-60° but decompose completely only above 300°. With triethylene qlycol (IV) or thiodiethylene qlycol (V) and tertiary alkanolamines in the presence of Cu salts, it prints cotton brilliant blue of excellent fastness to

light and washing. By suspending III 20.35 in EtOH 60, adding KOH 2.85 in EtOH 40, stirring a few hrs., filtering off KBr, and reducing the volume in vacuo, the free base (VI) 12 parts remains. It gives off NH3 at 120° and m. 160-5° (decomposition). A purer VI, m. 180-2°, can be obtained by dissolving III in H2O at 0-2°, adding a 7% NaOH solution, and filtering after a few min. Even at steam bath temperature, VI plus Cu salts give copper phthalocyanine in organic solvents like glycol or V. To EtOH 150 saturated with NH3, II 37.1 parts is added while cooling and the suspension is saturated with NH3. After stirring several hrs., NaOEt 20.4 parts in EtOH is added, stirring continued, the inorg, salt filtered off, the solution evaporated in vacuo, the residue redissolved in EtOH, filtered, and evaporated again to yield a yellow compound (VII) 12-14 parts producing brilliant blue prints in the presence of Cu salts. The 4-nitro derivative of I (VIII) 17.3 is stirred several hrs. with a 29% solution of HBr in AcOH 100 to give a thick precipitate 40 parts, which is filtered, washed with petr. ether, and dried in vacuo. The product (IX) decompose at about 200-10° and has the formula C8H6O2N3Br3. IX 41.6 is added with cooling to concentrated NH4OH 150 parts to give a yellow-green precipitate which is filtered and washed with a little H2O. Removing NH3 from the filtrate gives an addnl. yield. With Cu salts in glycol at 100° it produces a green dye. Printed in the presence of Cu salts, glycol, and triethanolamine it gives a green-blue dyeing of very good fastness. VIII replaced by the 4-chloro derivative of I gives a similar dye. The product from VII is pasted with V 2.5 and triethanolamine 0.5 and mixed with copper chloride 0.1 in H2O 1, incorporated into a 7% tragacanth solution 15 with the addition of a 60% solution of AcONH4 1 part to give a cotton printing paste. It produces brilliant blue dyeings after steaming 10 min., soaping, and rinsing. NiSO4 instead of CuCl2 produces a greener shade. The powder III is pasted with triethanolamine 0.5, V 1, and the triethanolamine salt of oleic acid 2, and mixed with a solution of copper chloride 0.1 in H2O 1 part. This mixture, pasted as above, gives a similar shade.

IT 574-93-6, Phthalocyanine

(derivs.)

T 91-15-6, Phthalonitrile

(derivs., and phthalocyanine compds. therefrom)

17654-68-1, Phthalonitrile, 4-chloro-

(dves from)

T 574-93-6, Phthalocyanine

(derivs.)

RN 574-93-6 CAPLUS

CN 29H, 31H-Phthalocyanine (CA INDEX NAME)



=> s (phthalocyanine OR "29H,31H-Phthalocyanine" OR "Porphyrins")

39709 PHTHALOCYANINE

7469 PHTHALOCYANINES

40559 PHTHALOCYANINE

```
(PHTHALOCYANINE OR PHTHALOCYANINES)
          1150 "29H"
          1184 "31H"
         39709 "PHTHALOCYANINE"
          7469 "PHTHALOCYANINES"
         40559 "PHTHALOCYANINE"
                 ("PHTHALOCYANINE" OR "PHTHALOCYANINES")
           919 "29H, 31H-PHTHALOCYANINE"
                 ("29H"(W)"31H"(W)"PHTHALOCYANINE")
         27345 "PORPHYRINS"
         66550 (PHTHALOCYANINE OR "29H, 31H-PHTHALOCYANINE" OR "PORPHYRINS")
=> s 112/prep
             0 PHTHALOCYANINE/CT
       4691145 PREP/RL
             0 PHTHALOCYANINE/PREP
                 (PHTHALOCYANINE/CT (L) PREP/RL)
             0 "29H, 31H-PHTHALOCYANINE"/CT
       4691145 PREP/RL
             0 "29H, 31H-PHTHALOCYANINE"/PREP
                 ("29H, 31H-PHTHALOCYANINE"/CT (L) PREP/RL)
         16446 "PORPHYRINS"/CT
       4691145 PREP/RL
          3028 "PORPHYRINS"/PREP
                 ("PORPHYRINS"/CT (L) PREP/RL)
          3028 ((PHTHALOCYANINE/PREP OR "29H, 31H-PHTHALOCYANINE"/PREP OR "PORPH
               YRINS"/PREP))
=> s 113 and metal-containing
       1888457 METAL
        940767 METALS
       2286478 METAL
                 (METAL OR METALS)
       696577 CONTAINING
             3 CONTAININGS
        696580 CONTAINING
                 (CONTAINING OR CONTAININGS)
       4290904 CONTG
            38 CONTGS
       4290916 CONTG
                 (CONTG OR CONTGS)
       4493882 CONTAINING
                 (CONTAINING OR CONTG)
         22430 METAL-CONTAINING
                 (METAL (W) CONTAINING)
             7 L13 AND METAL-CONTAINING
=> s 113 and (phthalonitrile OR "1,2-Benzenedicarbonitrile" OR "1,2-Dicyanobenzene"
OR "Phthalodinitrile")
          2233 PHTHALONITRILE
           340 PHTHALONITRILES
          2328 PHTHALONITRILE
                 (PHTHALONITRILE OR PHTHALONITRILES)
       9930505 "1"
       9870720 "2"
           778 "BENZENEDICARBONITRILE"
            28 "BENZENEDICARBONITRILES"
           786 "BENZENEDICARBONITRILE"
                 ("BENZENEDICARBONITRILE" OR "BENZENEDICARBONITRILES")
           453 "1,2-BENZENEDICARBONITRILE"
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L12

L13

T-14

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("1"(W)"2"(W)"BENZENEDICARBONITRILE")
      9930505 "1"
      9870720 "2"
         1388 "DICYANOBENZENE"
          136 "DICYANOBENZENES"
          1447 "DICYANOBENZENE"
                 ("DICYANOBENZENE" OR "DICYANOBENZENES")
           353 "1,2-DICYANOBENZENE"
                 ("1"(W)"2"(W)"DICYANOBENZENE")
           531 "PHTHALODINITRILE"
           44 "PHTHALODINITRILES"
           550 "PHTHALODINITRILE"
                 ("PHTHALODINITRILE" OR "PHTHALODINITRILES")
           26 L13 AND (PHTHALONITRILE OR "1,2-BENZENEDICARBONITRILE" OR "1,2-D
T.15
               ICYANOBENZENE" OR "PHTHALODINITRILE")
=> s 113 and (phthalonitrile OR "1,2-Benzenedicarbonitrile" OR "1,2-Dicyanobenzene"
OR "Phthalodinitrile")/ract
            0 PHTHALONITRILE/CT
       3206166 RACT/RL
             O PHTHALONITRILE/RACT
                (PHTHALONITRILE/CT (L) RACT/RL)
             0 "1,2-BENZENEDICARBONITRILE"/CT
       3206166 RACT/RL
             0 "1,2-BENZENEDICARBONITRILE"/RACT
                 ("1.2-BENZENEDICARBONITRILE"/CT (L) RACT/RL)
             0 "1,2-DICYANOBENZENE"/CT
       3206166 RACT/RL
             0 "1,2-DICYANOBENZENE"/RACT
                ("1,2-DICYANOBENZENE"/CT (L) RACT/RL)
             0 "PHTHALODINITRILE"/CT
      3206166 RACT/RL
             0 "PHTHALODINITRILE"/RACT
                ("PHTHALODINITRILE"/CT (L) RACT/RL)
L16
             0 L13 AND (PHTHALONITRILE OR "1,2-BENZENEDICARBONITRILE" OR "1,2-D
              ICYANOBENZENE" OR "PHTHALODINITRILE")/RACT
=> s 113 and alkoxy
        125108 ALKOXY
             7 ALKOXIES
        125114 ALKOXY
                 (ALKOXY OR ALKOXIES)
L17
            40 L13 AND ALKOXY
=> s 115 and alkoxy
        125108 ALKOXY
            7 ALKOXIES
        125114 ALKOXY
                (ALKOXY OR ALKOXIES)
1.18
            4 L15 AND ALKOXY
=> d 1-4 ibib hit hitstr abs
L18 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        2008:1251928 CAPLUS Full-text
DOCUMENT NUMBER:
                        149:474499
TITLE:
                        Silicon and germanium phthalocvanines and related
                        substances as fluorescent dyes and markers for liquid
                        products
INVENTOR(S):
                        Gessner, Thomas; Sens, Ruediger; Ahlers, Wolfgang;
```

Vamvakaris, Christos BASF SE, Germany

PCT Int. Appl., 79pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT ASSIGNEE(S):

SOURCE:

| PAT | ENT | NO. | | | KIN | D | DATE | | | APPL | ICAT | ION | NO. | | D | ATE | |
|------|------|------|------|-----|-----|-----|------|------|-----|------|------|------|-----|-----|-----|------|-----|
| | | | | | | - | | | | | | | | | | | |
| WO | 2008 | 1225 | 31 | | A2 | | 2008 | 1016 | | WO 2 | 008- | EP53 | 779 | | 2 | 0800 | 331 |
| | W: | ΑE, | AG, | AL, | AM, | AO, | AT, | AU, | ΑZ, | BA, | BB, | BG, | BH, | BR, | BW, | BY, | BΖ, |
| | | CA, | CH, | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DO, | DZ, | EC, | EE, | EG, | ES, |
| | | FI, | GB, | GD, | GE, | GH, | GM, | GT, | HN, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, |
| | | KG, | KM, | KN, | KΡ, | KR, | KZ, | LA, | LC, | LK, | LR, | LS, | LT, | LU, | LY, | MA, | MD, |
| | | ME, | MG, | MK, | MN, | MW, | MX, | MY, | MZ, | NA, | NG, | NI, | NO, | NZ, | OM, | PG, | PH, |
| | | PL, | PT, | RO, | RS, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SM, | SV, | SY, | TJ, | TM, |
| | | TN, | TR, | TT, | TZ, | UA, | UG, | US, | UZ, | VC, | VN, | ZA, | ZM, | ZW | | | |
| | RW: | AT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HR, | HU, |
| | | IE, | IS, | IT, | LT, | LU, | LV, | MC, | MT, | NL, | NO, | PL, | PT, | RO, | SE, | SI, | SK, |
| | | TR, | BF, | ВJ, | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | MR, | NE, | SN, | TD, |
| | | TG, | BW, | GH, | GM, | KE, | LS, | MW, | MZ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, |
| | | AM, | AZ, | BY, | KG, | ΚZ, | MD, | RU, | TJ, | TM | | | | | | | |
| RITY | APP | LN. | INFO | . : | | | | | | EP 2 | 007- | 1057 | 76 | - 1 | A 2 | 0070 | 405 |

PRIORITY APPLN. INFO.: OTHER SOURCE(S): MARPAT 149:474499 A 20070405

Silicon or germanium fused-ring-extended phthalocyanines are synthesized and used as tracer substances for liqs. and as markers for com. liqs. (especially fuels and petroleum products). The metallophthalocyanines are of general structure I, in which M1,M2, and M3 are Si or Ge; A, A1, A2, D, D1, D2, E,E1, E2, G,G1, and G2 are CH or N; n, m, p, and q are 0-2; 1 < n' < (4 + 2n), 1 <m' < (4 + 2m), 1 < p' < (4 + 2p), and 1 < q' < (4 + 2q); W, X, Y, Z, and R1-6,are halogen, nitro, hydroxy, cyano, amino, C1-20-alkyl, C2-20-alkenyl, C2-20alkynyl, C3-15-cycloalkyl, aryl, heterocyclic, C1-20-alkoxy, aryloxy, C1-4dialkylamino, C3-6-cycloalkylamino, -CO2M, -SO3M, and C1-4-dialkylsulfamoyl (M = H or alkali metal).

Porphyrins

RL: NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); PPEP (Preparation); USES (Uses)

(porphocyanins; silicon and germanium phthalocyanines and related substances as fluorescent dyes and markers for liquid products)

ΙT 76-86-8, Triphenylchlorosilane 91-15-6, 1,2-

Senzenedicarbonitrile 995-45-9, Tri-n-butvlchlorosilane 3634-67-1 18643-08-8, Octadecyldimethylchlorosilane 19333-15-4, Silicomphthalocyaninedihydroxide 52322-14-2 53175-37-4. 1-Amino-3-iminoisoindoline 162578-86-1 184719-55-9,

Chlorodiisopropyloctyloxy silane 859205-14-4, 3-(3-Methylpiperidino)

phthalodinitrile 1071438-03-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation reaction of; silicon and germanium phthalocyanines and related substances as fluorescent dyes and markers for liquid products)

^{*} STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AR Silicon or germanium fused-ring-extended phthalocyanines are synthesized and used as tracer substances for ligs. and as markers for com. ligs. (especially

fuels and petroleum products). The metallophthalocyanines are of general structure I, in which M1,M2, and M3 are Si or Ge; A, A1, A2, D, D1, D2, E,E1, E2, G,G1, and G2 are CH or N; n, m, p, and q are 0-2; $1 < n^1 < (4 + 2n)$, $1 < n^2 < (4 + 2p)$, and $1 < q^1 < (4 + 2q)$; W, X, Y, Z, and R1-6, are halogen, nitro, hydroxy, cyano, amino, C1-20-alky1, C2-20-alkeny1, C2-0-alky1, aryl, heterocyclic, C1-20-alkoxy, aryloxy, C1-4-dialkylamino, C3-6-cycloalkylamino, -CO2M, -SO3M, and C1-4-dialkylsulfamoy1 (M = H or alkali metal)

L18 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:1061593 CAPLUS Full-text

TITLE: Use of aryl- or alkyloxy-substituted phthalocyanines

as marking substances for liquids

INVENTOR(S): Gessner, Thomas; Ebert, Sophia; Sens, Ruediger; Koennemann, Martin; Ahlers, Wolfgang; Vamvakaris,

Christos

PATENT ASSIGNEE(S): Basf A.-G., Germany SOURCE: PCT Int. Appl., 53pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

| | TENT | | | | | | | | APPLICATION NO. | | | | | | | | |
|---------|--------|-------|------|-----|-------------|------|------|------|-----------------|-------|------|------|----------|-------|------|-------|------|
| WC | 2007 | 1046 | 85 | | A1 | | 2007 | 0920 | | WO 2 | 007- | EP52 | 122 | | 2 | 0070 | 307 |
| | W: | ΑE, | AG, | AL, | AM, | AT, | AU, | AZ, | BA, | BB, | BG, | BR, | BW, | BY, | BZ, | CA, | CH, |
| | | CN, | co, | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EC, | EE, | EG, | ES, | FI, | GB, | GD, |
| | | GE, | GH, | GM, | GT, | HN, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KM, | KN, |
| | | KP, | KR, | KZ, | LA, | LC, | LK, | LR, | LS, | LT, | LU, | LY, | MA, | MD, | MG, | MK, | MN, |
| | | MW, | MX, | MY, | MZ, | NA, | NG, | NI, | NO, | NZ, | OM, | PG, | PH, | PL, | PT, | RO, | RS, |
| | | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SM, | SV, | SY, | TJ, | TM, | TN, | TR, | TT, | TZ, |
| | | UA, | UG, | US, | UZ, | VC, | VN, | ZA, | ZM, | ZW | | | | | | | |
| | RW: | AT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HU, | IE, |
| | | IS, | IT, | LT, | LU, | LV, | MC, | MT, | NL, | PL, | PT, | RO, | SE, | SI, | SK, | TR, | BF, |
| | | BJ, | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | MR, | NE, | SN, | TD, | TG, | BW, |
| | | GH, | GM, | KE, | LS, | MW, | MZ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AM, | AZ, |
| | | BY, | KG, | KZ, | MD, | RU, | TJ, | TM | | | | | | | | | |
| AU | 2007 | 2245 | 12 | | A1 | | 2007 | 0920 | | AU 2 | 007- | 2245 | 12 | | 2 | 0070 | 307 |
| EF | 1996 | 549 | | | A1 20081203 | | | | | EP 2 | 007- | 7266 | 20070307 | | | | |
| | R: | AT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HU, | IE, |
| | | IS, | IT, | LI, | LT, | LU, | LV, | MC, | MT, | NL, | PL, | PT, | RO, | SE, | SI, | SK, | TR |
| PRIORIT | Y APP | LN. | INFO | . : | | | | | | EP 2 | 006- | 1111 | 61 | | A 2 | 0060 | 315 |
| | | | | | | | | | | WO 2 | 007- | EP52 | 122 | | W 2 | 0070 | 307 |
| OTHER S | OURCE | (S): | | | CASI | REAC | T 14 | 7:38 | 5765 | ; MAI | RPAT | 147 | :385 | 765 | | | |
| AB P | hthalo | ocyar | ines | 3 I | M = | н2, | Li2, | Mq, | Zn, | Cu, | Ni, | vo, | TiO |), Al | LC1, | A1 (C | Ac), |

AB Phthalocyanines I [M = H2, Li2, Mg, Zn, Cu, Ni, VO, TiO, AlCl, Al(OAc), AlCO(:0)OCF3, SiCl2, Si(OH)2; A = (R1)r; Q = (R)n; Z = (R)r; m = 1 - 4; n = 0 - 4; r = 0 - 4; m + r = 1 - 4; n + r = 0 - 4; R = OC(CRIRIR2)(CRIRIR1), X1, X2, X3, X4, X5, adamantyl-1-oxy; R1 = H, halogen, R2; R2 = Cl-18-alkyl, C4-eccolakyl, C2-12-alkkynl, C6-l0-aryl, (un)substituted C7-20-aralkyl (whereby the aryl is substituted with one or more halogen, CN, NO2, OH, NH2, Cl-20-alkyl (whereby the alkyl is optionally substituted with 1 - 4 O atoms), C1-20-alkyl (whereby the alkyl is optionally substituted with 1 - 4 O atoms), C1-20-alkyl optionally substituted with new properties of the complex of the complex optionally substituted with one or more halogens; s = R1; R3R3, R1R3 = ring system; R4, R5, R6 = H, halogen, Me, Et; Y1, Y2, Y3, Y4, Y5, Y6 = C1-4-alkylene, optionally substituted with one or more halogens; s =

0 - 6; t = 0 - 31 are suitable as marking substances for ligs., in particular

mineral oils. The preparation of I comprises: cyclocondensation of

```
phthalodinitriles II or iminoaminoisoindolines III or IV with a reducing agent in the presence of a base in a melt.
```

IT Nitriles, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
(dinitriles, phthalodinitriles, cyclocondensation reactions

of; use of ary1- or alkyloxy-substituted phthalocyanines as marking substances for ligs.)

IT Cyclocondensation reaction

(of phthalodinitriles or iminoisoindolines; use of aryl- or alkyloxy-substituted phthalocyanines as marking substances for liqs.)

IT Porphyrins

RL: PRP (Properties); SPN (Synthetic preparation); PREF (Preparation)

(phthalocyanines; use of aryl- or alkyloxy-substituted phthalocyanines as marking substances for ligs.)

166774-36-3P, 4-(1-Adamantanoxy)phthalodinitrile 214494-50-5P

214494-53-8P, 3-(2,6-Diisopropylphenoxy)phtbalodinitrile

214494-54-9P, 3-(2,6-Diphenylphenoxy)phthalodinitrile

 $651739-94-5P, \ 3-[2,4-Di(tert-pentyl)phenoxy] phthalodinirile$

949586-77-0P, 3-(2,4,6-Trimethylphenoxy)phthalodinitrile 949586-78-1P, 3-[4-(tert-Butyl)-2,6-diphenylphenoxy)

phthalodinitrile

Outumicainitaire

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation of; use of aryl- or alkyloxy-substituted phthalocyanines as marking substances for ligs.)

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Phthalocyanines I [M = H2, Li2, Mg, Zn, Cu, Ni, VO, TiO, AlCla, Al(OAC), AlCC(C:O)OCF3, SiCl2, Si(OH)2; A = (Rl)r; O = (R)n; Z = (R)m; m = 1 - 4; n = 0 - 4; r = 0 - 4; m + r = 1 - 4; n + r = 0 - 4; R = OC(CRIRIR) (CRIRIRI), XI, X2, X3, X4, X5, adamantyl-1-oxy; R1 = H, halogen, R2; R2 = Cl-18-alkyl, C4-8-cycloalkyl, C2-12-alkenyl, C2-12-alkynyl, C6-10-aryl, (un)substituted C7-20-aralkyl (whereby the aryl is substituted with one or more halogen, CN, NO2, OH, NH2, Cl-20-alkyl (whereby the alkyl is optionally substituted with 1 - 4 O atoms), C1-20-alkyl (whereby the alkyl is optionally substituted with 1 - 4 O atoms), C1-20-alkoylemino, C1-20-dialkylamino); E = (R3)t; R3 = R1; R3R3, R1R3 = ring system; R4, R5, R6 = H, halogen, Me, Et; Y1, Y2, Y3, Y4, Y5, Y6 = C1-4-alkylene, optionally substituted with one or more halogens; s = 0 - 6; t = 0 - 3] are suitable as marking substances for liqs.; in particular mineral oils. The preparation of I comprises: cyclocondensation of phthalodinitriles II or iminoaminoisoindolines III or IV with a reducing agent in the presence of a base in a melt.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2002:688155 CAPLUS Full-text DOCUMENT NUMBER: 137:241294

TITLE: Preparation of calixarene-substituted phthalocyanine derivatives as inclusion compounds and process for

preparation thereof

INVENTOR(S): Kuroda, Kazuyoshi; Kobayashi, Osao
Orient Chemical Industries, Ltd., Japan
SQURCE: Jpn. Kokai Tokkyo Koho, 21 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. JP 2002255968 20020911 JP 2001-58336 20010302 PRIORITY APPLN. INFO.: JP 2001-58336 20010302

OTHER SOURCE(S):

CASREACT 137:241294; MARPAT 137:241294 The title compds. [I; -X-L- represents a linkage group linked to calix[4] arene AB

at two adjacent β -positions of the aromatic ring of the phthalocyanine; X = 0, S; L = alkylene, -(CR4R5)q-Ar- (wherein R4, R5 = H, alkyl; Ar = arylene); R1, R2 = H, alkyl, aryl, aralkyl, halo; R3 = HO, alkoxy, acyloxy, aralkyloxy, thiol, thioalkoxy, OCH2(CH2)rCO2R6 (wherein R6 = H, alkyl; r = 0-2); M = two H atom, divalent metal atom, monosubstituted trivalent atom, disubstituted tetravalent atom; n = an integer of 1-4; * represents a linkage or substitution position] are prepared by reaction of 4,5-dichlorophthalonitrile and 3-mercaptopropanol, reaction of the resulting 4.5-bis(3-hydroxypropylthio) phthaionitrile with 4-tert-butylcalix[4]arene, and cycloaddn. reaction of the resulting calix[4]arene-substituted phthalonitrile followed by separation and purification and metal complexation. These compds. are inclusion compds. which possess a high degree of substitution, high symmetry, and fixed ligands and are useful as materials for fluorescence quenchers, gas sensors, sensitizers for laser phototherapy, photoelec. transducers, nonlinear optical devices, and optical recording materials. Thus, 8.0 part 4.5dichlorophthalonitrile and 8.6 part 3-mercaptopropanol were dissolved in 90 part DMSO, heated at 80°, treated with 90 part K2CO3 in 8 portions in every 5 min, and stirred at 80° for 30 min to give 58% 4,5-bis(3hydroxypropylthio)phahalomiarile which (7.3 part) was dissolved in 19 part pyridine, treated with p-toluenesulfonyl chloride at ≤5° in an ice-water, and stirred at the same temperature for 2 h to give 61% 4.5-bis(3tosyloxypropylthio)phthalonitrile (II). 4-Tert-butylcalix[4]arene 2.5, II 2.4, and K2CO3 1.3 part were added to 6 part acetone and refluxed for 30 h to give 19.0% 4-tert-butylcalix[4]arene-substituted phthalonitrile which (100 part) and 8.3 part DBU were added to 320 part 1-pentanol and refluxed for 24 h to give 5.9% tetrakis(4-tert-butylcalix[4]arene)-substituted phthalocyanine. Fluorescence quenching property of 1,4-benzoquinone due to the inclusion complexation with various calix[4]arene-substituted phthalocvanines was examined

ST calixarene substituted phthalocyanine prepn inclusion compd; cycloaddn calixarene substituted phthalonitrile

Metacyclophanes

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(calixarenes; preparation of calixarene-substituted phthalocvanine derivs. as inclusion compds. via cycloaddn. of calix[4]arene-substituted phthalonitrile)

Photosensitizers, pharmaceutical

(for laser phototherapy; preparation of calixarene-substituted phthalocyanine derivs, as inclusion compds, via cycloaddn, of calix[4]arene-substituted phthalonitrile)

Optical instruments

(nonlinear; preparation of calixarene-substituted phthalocyanine derivs. as inclusion compds. via cycloaddn. of calix[4]arene-substituted phthalonitrile)

ΙT Cycloaddition reaction

Gas sensors

Optical recording materials Photoelectric devices

IT Pornhyrine

RL: RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of calixarene-substituted phthalocyanine derivs. as inclusion compds. via cycloaddn. of calix[4]arene-substituted phthalonitrile)

IT Metalloporphyrins

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of calixarene-substituted phthalocyanine derivs. as inclusion compds. via cycloaddn. of calix[4]arene-substituted bythalonitriie)

IT Fluorescence

(quenchers; preparation of calixarene-substituted phthalocyanine derivs. as inclusion compds. via cycloaddn. of calix[4]arene-substituted phthalonitrile)

IT 106-51-4, 1,4-Benzoquinone, properties

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)

(inclusion complexation and fluorescence quenching of 1,4-benzoquinone; preparation of calixarene-substituted phthalocyanine derivs. as inclusion compds. via cycloaddn. of calix[4]arene-substituted phthalonitrile)

IT 459140-47-7P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(inclusion complexation and fluorescence quenching of 1,4-benzoquinone; preparation of calixarene-substituted phthalocyanine derivs. as inclusion compds. via cycloaddn. of calix[4]arene-substituted phthalonitriie)

T 459140-19-3P 459140-40-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (inclusion complexation and fluorescence quenching of 1,4-benzoquinone; preparation of calixarene-substituted phthalocyanine derivs. as inclusion compds, via cycloaddn. of calix[4]arene-substituted phthalonitrile)

IT 457901-24-5P 457901-25-6P 459125-82-PP 459125-83-8P 459125-84-9P
RI: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP
(Prevaration); RACT (Reactant) or reagent)

(preparation of calixarene-substituted phthalocyanine derivs. as inclusion compds. via cycloaddn. of calix[4]arene-substituted pbthalonitriie)

IT 98-59-9, p-Toluenesulfonyl chloride 7447-39-4, Copper(II) chloride,
reactions 7718-54-9, Nickel chloride, reactions 19721-22-3,
3-Mercaptopropanol 32703-80-3, 4-tert-Butylphthalonitrile 60705-62-6,
4-tert-Butylcalix(4)arene 139152-08-2, 4,5-Dichlorophthalonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of calixarene-substituted phthalocyanine derivs. as inclusion

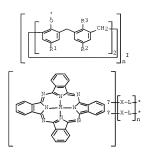
(preparation of calixarene-substituted phthalocyanine derivs. as inclusion compds. via cycloaddn. of calix[4]arene-substituted phthalonitrile)

IT 457901-22-3P, 4,5-Bis(3-hydroxypropylthio)phthalonitrile 457901-23-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of calixarene-substituted phthalocyanine derivs. as inclusion compds. via cycloaddn. of calix[4]arene-substituted

AB



at two adjacent β -positions of the aromatic ring of the phthalocyanine; X = 0, S; L = alkylene, -(CR4R5)g-Ar- (wherein R4, R5 = H, alkyl; Ar = arylene); R1, R2 = H, alkyl, aryl, aralkyl, halo; R3 = HO, alkoxy, acyloxy, aralkyloxy, thiol, thioalkoxy, OCH2(CH2)rCO2R6 (wherein R6 = H, alkyl; r = 0-2); M = two H atom, divalent metal atom, monosubstituted trivalent atom, disubstituted tetravalent atom; n = an integer of 1-4; * represents a linkage or substitution position] are prepared by reaction of 4,5-dichlorophthalonitrile and 3-mercaptopropanol, reaction of the resulting 4,5-bis(3-hydroxypropylthio) phthalonitrile with 4-tert-butylcalix[4]arene, and cycloaddn. reaction of the resulting calix[4]arene-substituted phthalonitrile followed by separation and purification and metal complexation. These compds. are inclusion compds. which possess a high degree of substitution, high symmetry, and fixed ligands and are useful as materials for fluorescence quenchers, gas sensors, sensitizers for laser phototherapy, photoelec. transducers, nonlinear optical devices, and optical recording materials. Thus, 8.0 part 4,5dichlorophthalonitrile and 8.6 part 3-mercaptopropanol were dissolved in 90 part DMSO, heated at 80°, treated with 90 part K2CO3 in 8 portions in every 5 min, and stirred at 80° for 30 min to give 58% 4,5-bis(3hydroxypropylthio)phthalonitrile which (7.3 part) was dissolved in 19 part pyridine, treated with p-toluenesulfonvl chloride at ≤5° in an ice-water, and stirred at the same temperature for 2 h to give 61% 4,5-bis(3tosyloxypropylthio)phthalonitrile (II). 4-Tert-butylcalix[4]arene 2.5, II 2.4, and K2CO3 1.3 part were added to 6 part acetone and refluxed for 30 h to give 19.0% 4-tert-butylcalix[4]arene-substituted phthalonitrile which (100 part) and 8.3 part DBU were added to 320 part 1-pentanol and refluxed for 24 h to give 5.9% tetrakis(4-tert-butylcalix[4]arene)-substituted phthalocyanine. Fluorescence quenching property of 1,4-benzoquinone due to the inclusion complexation with various calix[4]arene-substituted phthalocyanines was examined

The title compds. [I; -X-L- represents a linkage group linked to calix[4] arene

L18 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1994:536221 CAPLUS Full-text

DOCUMENT NUMBER: 121:136221

ORIGINAL REFERENCE NO.: 121:24625a,24628a
TITLE: Preparation of phthalocyanine derivatives and

intermediates thereof

INVENTOR(S): Fujiwara, Koji; Kudo, Masaaki; Akita, Takavuki

PATENT ASSIGNEE(S): Nihon Nohyaku Co Ltd, Japan SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE ____ JP 06041137 A 19940215 JP 1993-43181 19930208 PRIORITY APPLN. INFO.: JP 1992-56895 A1 19920208 OTHER SOURCE(S): CASREACT 121:136221; MARPAT 121:136221 Phthalocyanine derivs. [I; R = lower (halo)alkyl, (halo)alkoxy, or

(halo)alkylthio, particularly CF3; n = 0-4] are prepared by reaction of dichlorobenzene derivs. (II; X = C1; R, n = same as above) with C0 and inorg. ammonium salt in the presence of a Fd compound and a phosphine compound, reaction of the resulting phthalimide derivs. (III; R, n = same as above) with NH3, treatment of the resulting phthalamide derivs. II (X = C0NH2; R, n = same as above) with P(O)Cl3, and reaction of the resulting phthalonitriles II (X = cvano; R, n = same as above) with a metal oxide or halide in the presence of a

basic catalyst. They are useful as dyes and functional materials. Thus, 3,4-dichlorobenzotrifluoride 0.18, NH4HCO3 0.56, PdCl2 0.0018, 1,4-bis(diphenylphosphino)butane 0.09 mol, and 180 mL toluene were placed in a Hastelloy autoclave, purged three times with CO (5 kg/cm2), pressurized with CO (35 kg/cm2), and allowed to react at 200° for 3 h to give 65.6% 4-

trifluoromethylphthalimide. The latter compound was stirred with 28% aqueous NH3 at room temperature to give 82.1% 4-trifluoromethylphthalamide which was dissolved in pyridine, cooled to 5°, and treated dropwise with P(O)Cl3 followed by heating at 60° for 2 h to give 72.8% 4-

trifluoromethylphthalonitrile. The latter nitrile 0.98, SnCl2 0.28, and DBU

0.76 were refluxed in EtCCHZCHZOH for 6 h and cooled followed by adding water and filtering precipitated crystals to give 100 N [(R = CF3, n = 1, M = Sn). Cvcloaddition reaction

IT Cycloaddition reaction

(of phthalonitriles in presence of metal oxides or metal halides, metal phthalocyanines from)

IT Porphyrins

RL: IMF (Industrial manufacture); PREP (Preparation)
(metal complexes, preparation of, by cycloaddn. of phthalonitriles

in presence of meta halides or oxides)

$$(R)_{n}$$

$$(R)_$$

dichlorobenzene derivs. (II; X = Cl; R, n = same as above) with CO and inorg. ammonium salt in the presence of a Pd compound and a phosphine compound, reaction of the resulting phthalimide derivs. (III; R, n = same as above) with NH3, treatment of the resulting phthalamide derivs. II (X = CONH2; R, n = same as above) with P(0)C13, and reaction of the resulting phthaionitriles II (X = cyano; R, n = same as above) with a metal oxide or halide in the presence of a basic catalyst. They are useful as dyes and functional materials. Thus, 3.4dichlorobenzotrifluoride 0.18, NH4HCO3 0.56, PdCl2 0.0018, 1,4bis(diphenylphosphino)butane 0.09 mol, and 180 mL toluene were placed in a Hastelloy autoclave, purged three times with CO (5 kg/cm2), pressurized with CO (35 kg/cm2), and allowed to react at 200° for 3 h to give 65.6% 4trifluoromethylphthalimide. The latter compound was stirred with 28% aqueous NH3 at room temperature to give 82.1% 4-trifluoromethylphthalamide which was dissolved in pyridine, cooled to 5°, and treated dropwise with P(0)C13 followed by heating at 60° for 2 h to give 72.8% 4trifluoromethylphthalonitrile. The latter nitrile 0.98, SnCl2 0.28, and DBU 0.76 were refluxed in EtOCH2CH2OH for 6 h and cooled followed by adding water and filtering precipitated crystals to give 100% I (R = CF3, n = 1, M = Sn).

Phthalocyanine derivs. [I; R = lower (halo)alkyl, (halo)alkoxy, or (halo)alkylthio, particularly CF3; n = 0-4] are prepared by reaction of

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E PHTHALOCYANINE/CN

1 S E3

FILE 'CAPLUS' ENTERED AT 13:22:37 ON 19 DEC 2008 L2 8782 S L1

FILE 'REGISTRY' ENTERED AT 13:24:15 ON 19 DEC 2008

FILE 'CAPLUS' ENTERED AT 13:24:33 ON 19 DEC 2008

1.3 3519 S L1 AND METAL L4 0 S L3/PREP

L5 998 S L1/PREP

L6 156 S L5 AND PHTHALONITRILE 1.7 25 S L5 AND ALKOXY

L8 79 S L1 AND METAL-CONTAINING

0 S L8/PREP L9

L10 6 S L8 AND PHTHALONITRILE SET LINE 250

SET DETAIL OFF E PHTHALONITRILE+ALL/CT SET LINE LOGIN SET DETAIL LOGIN

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L11
              7 S L8 AND (PHTHALONITRILE OR "1,2-BENZENEDICARBONITRILE" OR "1,2
               SET LINE 250
                SET DETAIL OFF
                E PHTHALOCYANINE+ALL/CT
                SET LINE LOGIN
                SET DETAIL LOGIN
         66550 S (PHTHALOCYANINE OR "29H.31H-PHTHALOCYANINE" OR "PORPHYRINS")
L12
L13
           3028 S L12/PREP
L14
              7 S L13 AND METAL-CONTAINING
                SET LINE 250
                SET DETAIL OFF
                E PHTHALONITRILE+ALL/CT
                SET LINE LOGIN
                SET DETAIL LOGIN
L15
            26 S L13 AND (PHTHALONITRILE OR "1,2-BENZENEDICARBONITRILE" OR "1,
                SET LINE 250
                SET DETAIL OFF
                E PHTHALONITRILE+ALL/CT
                SET LINE LOGIN
                SET DETAIL LOGIN
1.16
             0 S L13 AND (PHTHALONITRILE OR "1,2-BENZENEDICARBONITRILE" OR "1,
L17
             40 S L13 AND ALKOXY
L18
              4 S L15 AND ALKOXY
     FILE 'STNGUIDE' ENTERED AT 13:43:51 ON 19 DEC 2008
                SET LINE 250
                SET DETAIL OFF
                SAVE L1, L2, L3, L5, L6, L7, L8, L10, L11, L12, L13, L14, L15, L17, L18 STN10
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                SET DETAIL LOGIN
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=> LOG H
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     FILE 'REGISTRY' ENTERED AT 13:21:06 ON 19 DEC 2008
               E PHTHALOCYANINE/CN
              1 SEA SPE=ON ABB=ON PLU=ON PHTHALOCYANINE/CN
                D SCAN
     FILE 'CAPLUS' ENTERED AT 13:22:37 ON 19 DEC 2008
           8782 SEA SPE=ON ABB=ON PLU=ON L1
L2
     FILE 'REGISTRY' ENTERED AT 13:24:15 ON 19 DEC 2008
                D L1 1 IDE
    FILE 'CAPLUS' ENTERED AT 13:24:33 ON 19 DEC 2008
L3
           3519 SEA SPE=ON ABB=ON PLU=ON L1 AND METAL
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0 SEA SPE-ON ABB-ON PLU-ON (L1 AND METAL/PREP)
T.4
L5
          998 SEA SPE=ON ABB=ON PLU=ON L1/PREP
          156 SEA SPE=ON ABB=ON PLU=ON L5 AND PHTHALONITRILE
L6
L7
           25 SEA SPE=ON ABB=ON PLU=ON L5 AND ALKOXY
L8
            79 SEA SPE=ON ABB=ON PLU=ON L1 AND METAL-CONTAINING
1.9
             0 SEA SPE=ON ABB=ON PLU=ON (L1 AND METAL-CONTAINING/PREP)
             6 SEA SPE=ON ABB=ON PLU=ON L8 AND PHTHALONITRILE
L10
               SET LINE 250
               SET DETAIL OFF
               E PHTHALONITRILE+ALL/CT
               SET LINE LOGIN
               SET DETAIL LOGIN
1.11
             7 SEA SPE=ON ABB=ON PLU=ON L8 AND (PHTHALONITRILE OR "1.2-BENZ
               ENEDICARBONITRILE" OR "1,2-DICYANOBENZENE" OR "PHTHALODINITRILE
               ")
               D IBIB HIT HITSTR
               D 2-6 IRIB HIT HITSTR
               SET LINE 250
               SET DETAIL OFF
               E PHTHALOCYANINE+ALL/CT
               SET LINE LOGIN
               SET DETAIL LOGIN
L12
        66550 SEA SPE=ON ABB=ON PLU=ON (PHTHALOCYANINE OR "29H, 31H-PHTHALO
               CYANINE" OR "PORPHYRINS")
          3028 SEA SPE=ON ABB=ON PLU=ON ((PHTHALOCYANINE/PREP OR "29H,31H-P
L13
               HTHALOCYANINE"/PREP OR "PORPHYRINS"/PREP))
L14
             7 SEA SPE=ON ABB=ON PLU=ON L13 AND METAL-CONTAINING
               SET LINE 250
               SET DETAIL OFF
               E PHTHALONITRILE+ALL/CT
               SET LINE LOGIN
               SET DETAIL LOGIN
L15
            26 SEA SPE=ON ABB=ON PLU=ON L13 AND (PHTHALONITRILE OR
               "1,2-BENZENEDICARBONITRILE" OR "1,2-DICYANOBENZENE" OR
               "PHTHALODINITRILE")
               SET LINE 250
               SET DETAIL OFF
               E PHTHALONITRILE+ALL/CT
               SET LINE LOGIN
               SET DETAIL LOGIN
L16
             O SEA SPE=ON ABB=ON PLU=ON L13 AND (PHTHALONITRILE OR
               "1,2-BENZENEDICARBONITRILE" OR "1,2-DICYANOBENZENE" OR
               "PHTHALODINITRILE")/RACT
            40 SEA SPE=ON ABB=ON PLU=ON L13 AND ALKOXY
L18
             4 SEA SPE=ON ABB=ON PLU=ON L15 AND ALKOXY
               D 1-4 IBIB HIT HITSTR ABS
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